Storage Needs for GENIE

Gabriel Perdue Fermilab 2014/September/3





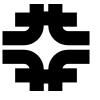




GENIE

- Generates Events for Neutrino Interaction Experiments.
- http://genie.hepforge.org
- Well-engineered C++ software framework built on sound 00principles and design patterns. (The Gang of Four is omnipresent.)
- Propagates a flux of neutrinos (specified by function, histogram, or ntuple) through a geometry (Geant4– compatible) and simulates the initial interaction and propagation of hard vertex products through the nuclear medium. Geant4 takes over when particles leave the nucleus.
- ROOT provides many core utilities. GENIE also heavily leverages other HEP and FOS software — LHAPDF, GSL, Pythia, log4cpp, etc.

Andreopoulos, C. and Bell, A. and Bhattacharya, D. and Cavanna, F. and Dobson, J. and others. "The GENIE Neutrino Monte Carlo Generator". Nucl.Instrum.Meth. A614. 87-104. 2010.





GENIE at FNAL

- GENIE is the primary event generator for:
 - ArgoNeut
 - LAr1-ND
 - LBNE
 - MicroBooNE
 - MINERVA
 - NOvA
- GENIE is also being considered for special studies by MINOS and MiniBooNE (they use previous generation software for their main generators).





Software Dependencies

- GENIE uses ROOT (5, eventually 6), Pythia(6, eventually 8), LHAPDF (5, eventually 6), log4cpp, GSL.
- Libraries: libstdc++, libc, libgcc, linux-vdso, libm, ld-linux-x86-64, libxml2 ... possibly not complete (ROOT, etc. have requirements).
- GENIE does not (yet) use any features from C++11.
- Generally, building on Scientific Linux is easy.
- Building 32-bit is also possible.





> ./cloc-1.60.pl R-2_8_0/
 3285 text files.
 3200 unique files.
 7197 files ignored.

http://cloc.sourceforge.net v 1.60 T=113.14 s (11.3 files/s, 4119.1 lines/s)

| Language | files | blank | comment | code |
|--------------------|-------|-------|---------|--------|
| C++ | 525 | 30478 | 37587 | 176349 |
| XML | 125 | 21895 | 2144 | 147176 |
| C/C++ Header | 504 | 9052 | 8118 | 22282 |
| Perl | 28 | 456 | 1469 | 3620 |
| make | 47 | 514 | 485 | 1651 |
| Bourne Shell | 34 | 157 | 334 | 1059 |
| Bourne Again Shell | 2 | 145 | 127 | 727 |
| SQL | 12 | 37 | 0 | 117 |
| SUM: | 1277 | 62734 | 50264 | 352981 |

There is a lot of configuration XML and experimental data packaged for the validation framework.





Development Needs

- GENIE requires ~250 MB (uncompressed) for its code and libraries, plus ~2 GB of third party code that will change rarely (85% is ROOT).
 - This may actually be more like ~10 GB if we keep many different versions of ROOT.
- Four core developers at the lab, plus 5-10 "moonlighters" from the experiments.
 - I keep, for example, almost 10 different versions of GENIE in my MINERvA working area.
- Storage requirements for development (not production!) is less than 100 GB per developer (justification follows).
- A "small" 5 TB BlueArc allocation would probably cover development needs for the foreseeable future.





Validation Needs

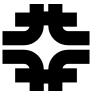
- Significantly more complicated storage picture.
 - Discuss "high-level" needs only here...
- The initial goal is to run the validation weekly.
- We would like to work towards a more rapid cycle, perhaps daily. This is less for development and more for...
- We would like to eventually be able to use these "validation runs" to do physics tuning.
 - This would require designing a compressed validation so that it could be run several times per day.





Scripting Framework

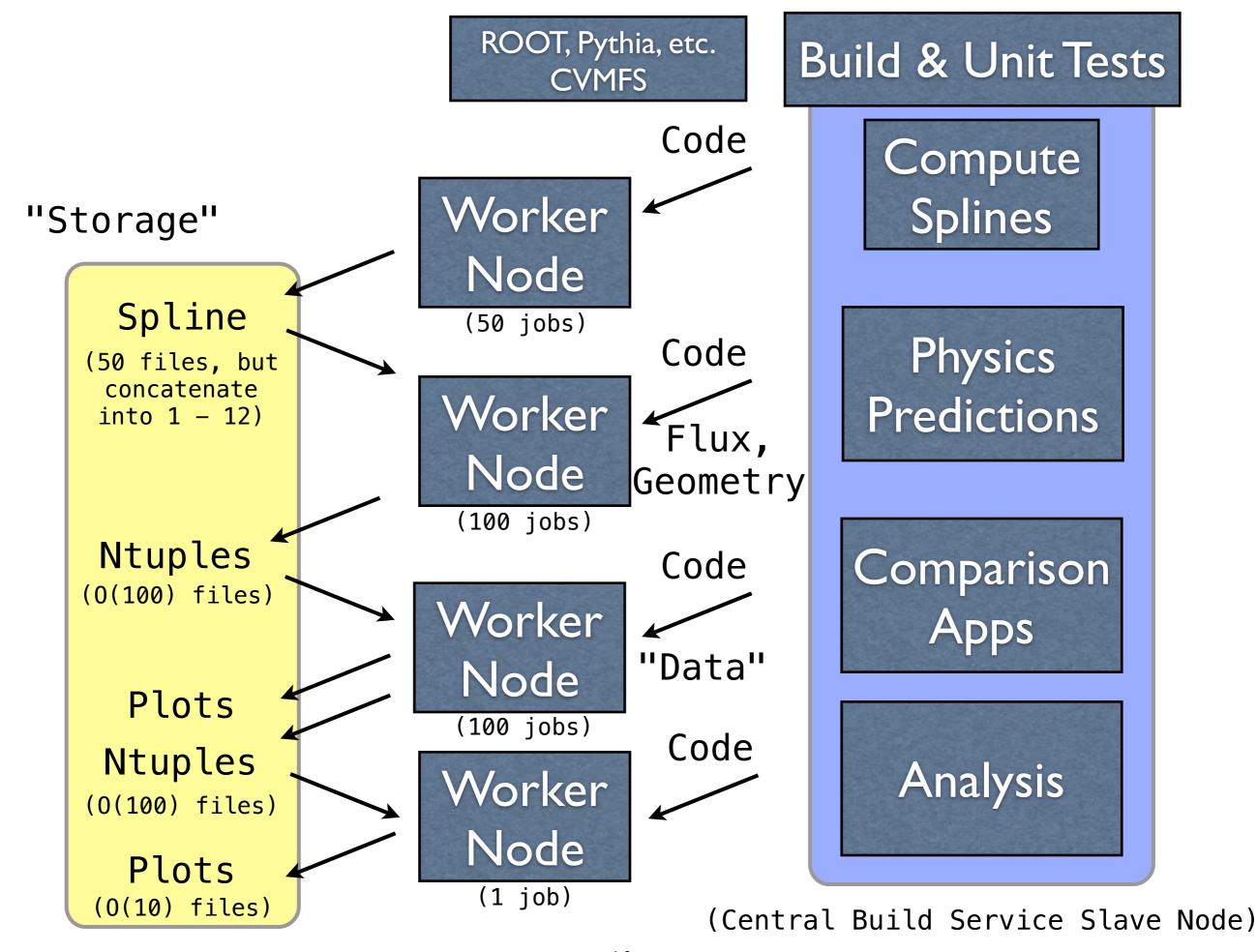
- Six Stages:
 - Build
 - Unit Tests (Eventually)
 - Generate Cross Sections (In: NA; Out: XML)
 - Generate Physics Predictions (In: XML, Geometry, Flux; Out: ROOT Ntuples)
 - Run Data/MC Comparison Apps (In ROOT Ntuples; Out ROOT Ntuples, PDFs)
 - Compare outputs to previous data/MC comparisons / Study global behavior (In ROOT Ntuples; Out ROOT Ntuples, PDFs)
- Each step depends on the previous step succeeding.
- We plan on using the Central Build Service to coordinate the flow from one stage to the next, but each stage will have its own script.
 - Working with LArSoft on this there may be only one or two scripts, but instead each stage will be controlled by a different configuration file.

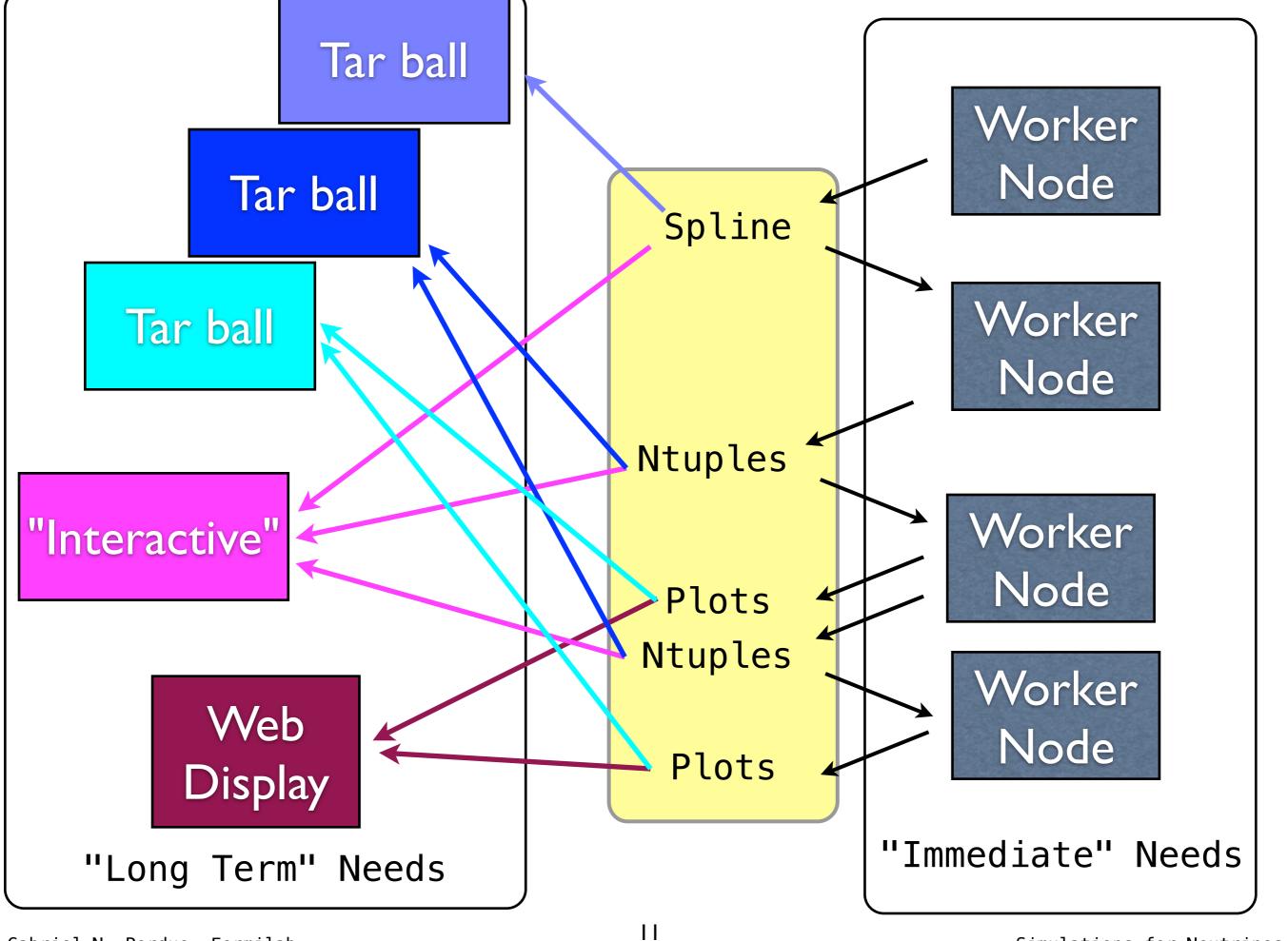


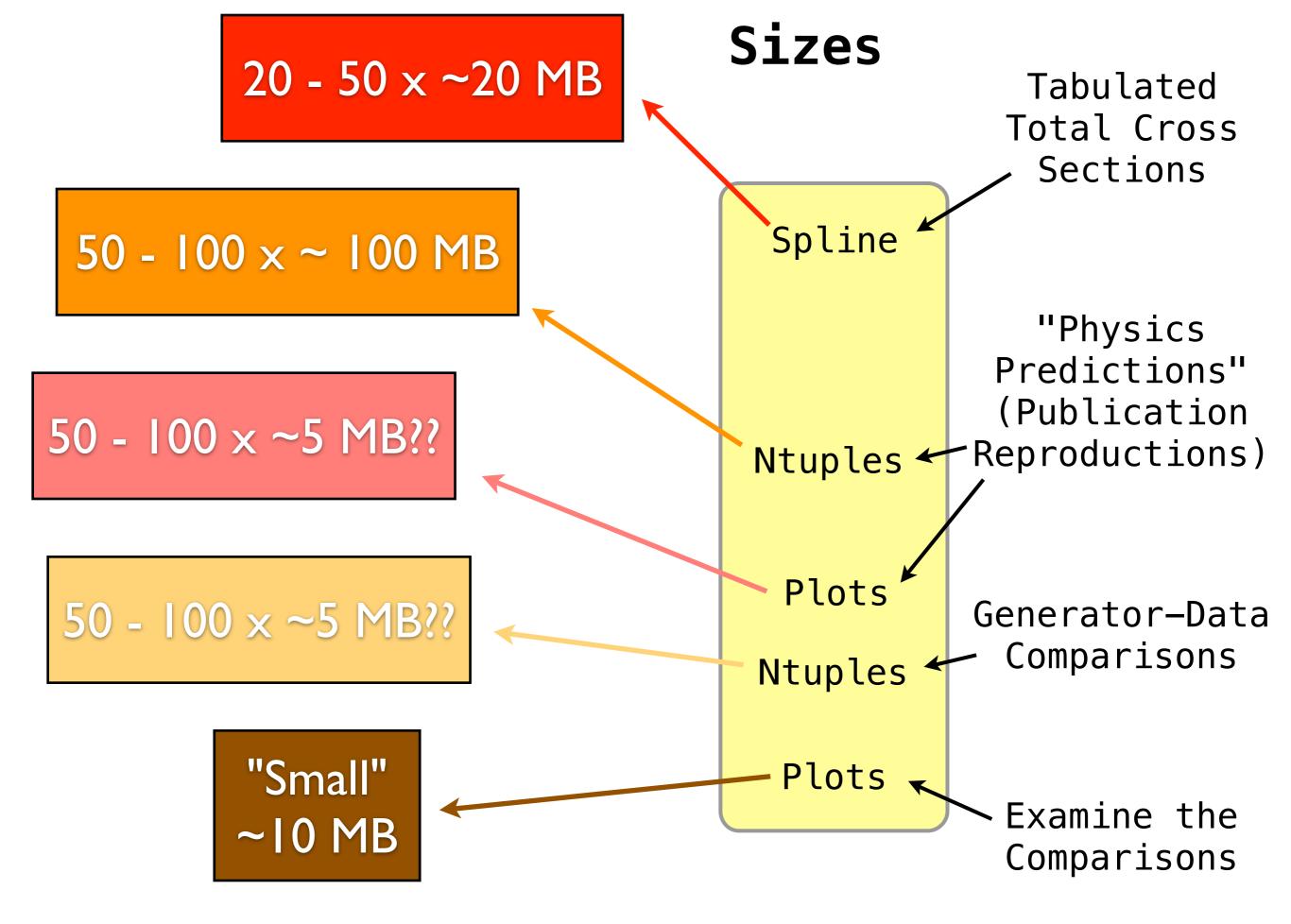


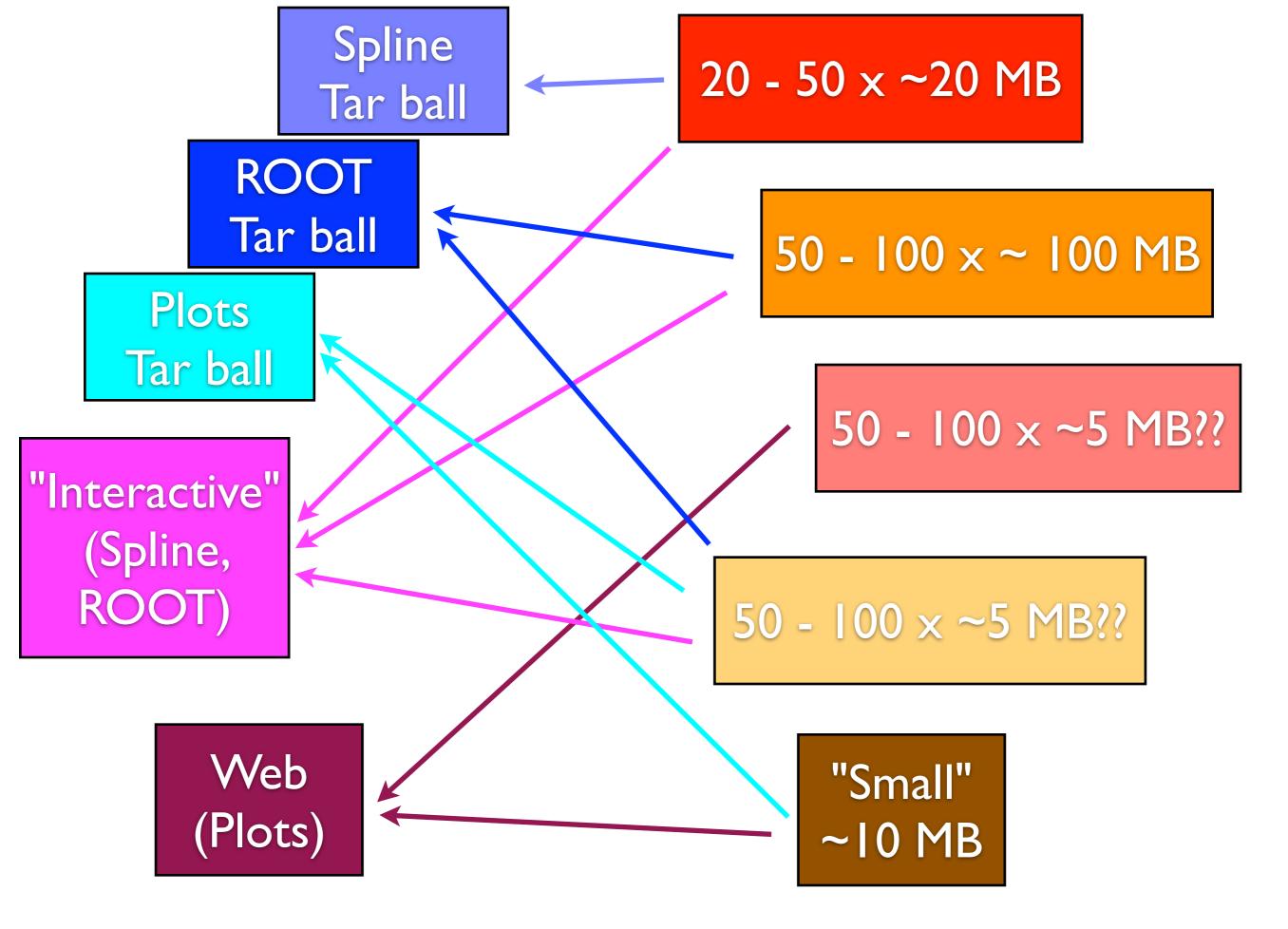
Scripting Framework

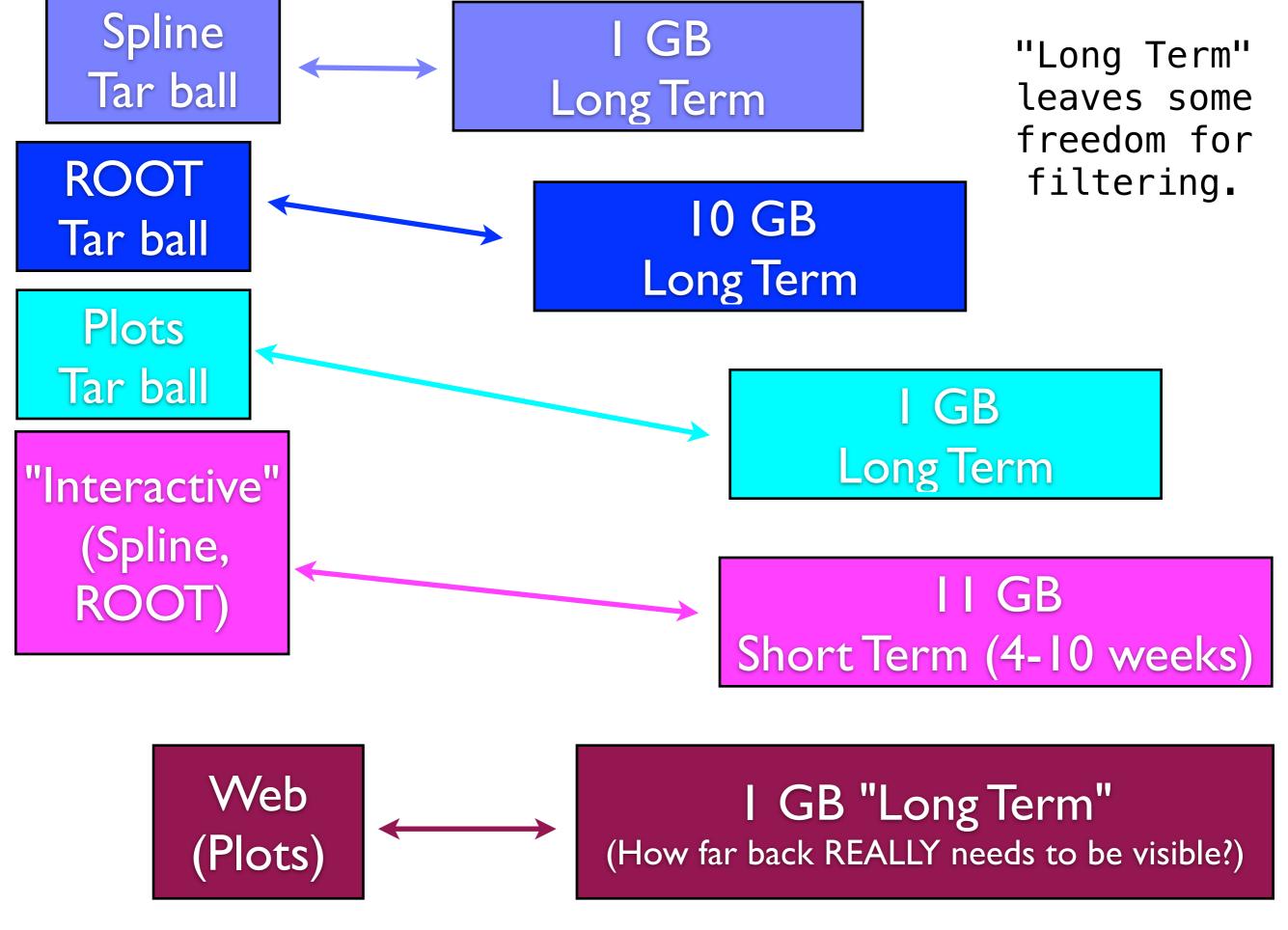
- Build
 - GENIE: 250 MB
 - 3rd Party (Pythia, LHAPDF, ROOT, GSL, log4cpp): 2 GB
 - Infrequent changes (so use CVMFS), but may want multiple copies of ROOT.
- Generate Cross Sections (In: NA; Out: XML)
 - Output size: ~1 GB (can vary by 1 order of magnitude based on number of targets, number of knots in the spline); Run time: ~12 hours per job (upper bound - light nuclei are much faster than heavy nuclei).
- Generate Physics Predictions & Run Data/MC Comparison Apps
 - Output size: ~100's of MB per App. Only a handful of apps on day one. (Several dozen are "available." Plan to make many more.) Total storage: ~10 GB; Run time: ~several hours per job.
- Compare outputs to previous data/MC comparisons / Study global behavior (In ROOT Ntuples; Out ROOT Ntuples, PDFs)
 - Vaporware today... estimated output is small (summary plots must be human consumable).















Aggregation and Tracking

- What is the aggregate request?
 - There is some flexibility if there is less space we will filter older files more aggressively.
 - We want to keep *release* validation "forever" but this is small (100 GB per release is very conservative).
 - For tuning we may want to keep many dozens of copies of varied validation, but the timescale for retention would be short (weeks) and the long-term storage could be highly filtered and compressed.





- Suppose we wanted to keep 1000 validation cycles.
 - 10 TB
 - The main complications are:
 - File sizes for new validation apps could be quite large.
 - We may want to do many cycles when tuning.
 - Juggling files into the tape archive.





- Book-keeping
 - Ideally we heavily leverage SAM.
 - What do we need to do on the GENIE end to make this possible?





Timeline

- The goal is to complete the validation framework by next Summer.
 - We will continue to develop validation and tuning applications for years, but the framework should be able to accommodate additional apps with no changes.





More Detailed Stage Discussion





Build

- Script in hand that does green-field builds with minimal checks for previously installed 3rd party codes.
- Currently assumes x86_64.
- Not CVMFS aware.
- Bash. Willing to rewrite into Python it is missing some functionality anyway, e.g., how to declare files to SAM, etc.
 - Requires Git, wget, gcc 4.1+ (can probably go lower), gfortran, Python (2.6?) for the full stack (ROOT + Pythia6 + LHAPDF5).

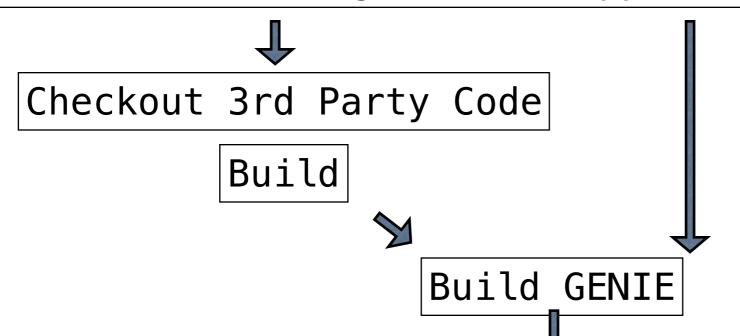


Specify Config: GENIE, 3rd Party Code Versions



Checkout GENIE

Check for versioned 3rd Party Code
 (in /grid/fermiapp or CVMFS)



Declare binaries/ libraries to SAM?

Install GENIE - /grid/fermiapp/pds/genie

Report Success 0
Failed Checkout 1
Failed 3rd Party Build 2
Failed 3rd Party Find 3
Failed 3rd Party Installation 4
Failed GENIE Build 5
Failed GENIE Installation 6

Declare data sets
/ support files
to SAM





Generate Cross Sections

- "Bootstrap Option": Keep a set of splines in /pnfs/data(?) for testing other components of the scripting framework.
- Comparison: Store a complete set of splines from official releases, the last X validation releases (where X is probably one for automated comparisons).
- ~20-50 grid jobs if we do one job per target (could choose to break up the Event Generator Lists).
- Output at this stage is $\sim 20-50 \times \sim 20$ MB files, which could be concatenated into a smaller set of files (or one file).
 - One for free nucleons, one for each element (favorites: He, C, O, N, Ar, Fe, etc. Minerva has ~20.).
- Jobs in the next stage must load the file, and the inefficiency in loading unneeded cross sections is outweighed by simpler coordination.



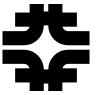


gmkspl

- GENIE Make Spline
- Example:

```
$ gmkspl -p 14,-14 -t 1000060120 -o carbon_splines.xml \
--event-generator-list Default
```

- Set the Projectile (PDG code), the Target (PDG Ion Code), the output, and the Event Generator List.
- The `Default` list contains 13 generator lists (CCQE, COH, DIS, etc.).
- Each generator list contains from one to three (roughly) cross section models.







```
<?xml version="1.0" encoding="ISO-8859-1"?>
     <!-- generated by genie::XSecSplineList::SaveSplineList() -->
     <genie_xsec_spline_list version="2.00" uselog="1">
                        Cross Section Algorithm
                                                           Neutrino Flavor (PDG Code)
     <spline</pre>
         name="genie: LwlynSmithQELCCPXSecyDefault nu:-14;"
Target
        tgt:1000060120;
(Carbon)
         N:2212;
         proc:Weak[CC],QES;"
         nknots="44">
       <knot> <E> 0.01000 </E> <xsec>
                                                0 </xsec> </knot>
       <knot> <E> 0.030466 </E> <xsec>
                                                  0 </xsec> </knot>
       <knot> <E> 0.050932 </E> <xsec>
                                                  0 </xsec> </knot>
       <knot> <E> 0.071399 </E> <xsec>
                                                  0 </xsec> </knot>
                    0.091865 </E> <xsec>
       <knot> <E>
                                                  0 </xsec> </knot>
       <knot> <E>
                     0.11233 </E> <xsec>
                                                  0 </xsec> </knot>
                      0.1427 </E> <xsec> 8.487371629e-13 </xsec> </knot>
       <knot> <E>
       <knot> <E>
                     0.18129 </E> <xsec> 4.103713443e-12 </xsec> </knot>
       <knot> <E> 0.2303 </E> <xsec> 8.367696679e-12 </xsec> </knot>
                     0.29257 </E> <xsec> 1.290439962e-11 </xsec> </knot>
       <knot> <E>
       <knot> <E>
                     0.37168 </E> <xsec> 1.807792243e-11 </xsec> </knot>
       . . .
                                               Cross Section
                     Energy (GeV)
                                                   (GeV^{-2})
```



Specify Config: List of targets, List of Event Generator Lists per target, code location





For each target material:

For each target Event Generator List:



Run `gmkspl` as a grid job.



Once all of the splines are finished, concatenate them, store the concatenated file in /pnfs(?); Declare concatenated output only to FTS/SAM?

Report Success 0 Failed to find Code 1 Failed to concatenate and store 2 Failed on Target <PDG Code>





Generate Physics Predictions

- Each prediction is a unique snowflake.
- Requires the cross section spline and support files: a flux and target specification (likely to complicated, but small):
 - e.g., the NuMI flux on the MINERvA geometry
 - Sometimes very simple, e.g. 500 MeV electrons on carbon





Specify Config: List of predictions, code location, support files location paired with prediction (traditionally with the code); here each app will ask SAM for support files.



For each application:



Run its script (may be complicated, may be Bash, Python, Perl, etc.) as a grid job



As each of the apps are finished, store the output file in /pnfs(?) & Declare to FTS/SAM

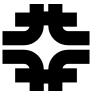
Report Success 0 Failed to store output 1 Failed on finish app <App Code>





Comparison Applications

- Each application is a unique snowflake.
- Requires a published data set and the generator predictions file.
- Jobs should be very fast (unless they are doing a complicated fit, etc.).
- Output is plots and ROOT files (histograms and/or ntuples).





Specify Config: List of applications, paired list of data set and generator prediction files (each app will ask SAM for data set and prediction set)



For each application:



Run its script (may be complicated, may be Bash, Python, Perl, etc.) as a grid job



As each of the apps are finished, store the output file in /pnfs(?) Ntuples+Historgrams to BlueArc, Plots+ROOT files to /pnfs(?)

Report Success 0 Failed to finish app <App Code>